

Time-local unraveling of non-Markovian stochastic Schrödinger equations

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Non-Markovian stochastic Schrödinger equations (NMSSE) are an important tool in quantum mechanics, from the theory of open systems to foundations. Yet, in general, they are but formal objects: their solution can be computed numerically only for some classes of non-trivial systems. We propose to write the stochastic realizations of NMSSE as averages over the solutions of an auxiliary equation with an additional random field. Our method yields non-perturbative numerical simulation algorithm for generic NMSSE that can be made arbitrarily accurate for reasonably short times.

I. INTRODUCTION

Stochastic pure state representations have a wide range of applications in quantum mechanics: they serve as computational tools to unravel open-system evolutions, as modelling tools to describe continuous measurement situations and as foundational tools to solve the measurement problem in models where the superposition principle breaks down. In the Markovian limit, the solutions of stochastic Schrödinger equations can be efficiently computed numerically, justifying their wide use in the three aforementioned fields. In the non-Markovian case however, there exists no general purpose method to compute a realization of the random pure state process: plotting a single trajectory is in general impossible. In this article, we propose to write the solutions of general stochastic Schrödinger equations as averages over the solutions of time-local stochastic Schrödinger equations with an auxiliary noise. We shall use the same trick that usually allows to replace openness by stochasticity, this time to get rid of non-Markovianity.

Although stochastic Schrödinger equations have a long history dating back to the eighties [1, 2], the field took off when their potential in numerics was understood by Dalibard, Castin and Mølmer [3, 4] (see also Dum, Zoller and Ritsch [5]) in the jump case and by Gisin and Percival [6] in the diffusive case. The connection with actual quantum trajectories coming from realistic measurement setups was understood roughly at the same time by Milburn and Wiseman [7] (see *e.g.* [8] for an introduction). Interestingly, the introduction of continuous stochastic pure state equations in foundations is slightly anterior with the Continuous Spontaneous Localization (CSL) model of Pearle, Ghirardi and Rimini [9, 10] and the gravity related collapse model of Diósi [11], both aimed at solving the measurement problem (see [12, 13] for a review). The generalization of the formalism to the non-Markovian realm was carried out by Diósi and Strunz [14, 15]. In that case, the measurement interpretation exists but is admittedly more subtle: a given trajectory only has a local point by point measurement interpretation [16] but no real time meaning [17–19], at least

within orthodox interpretations of the formalism [20]. Non-Markovian stochastic approaches have also infected foundations with various extensions of the initial CSL proposal [21, 22]. In all these applications, the practical problem is always the same: the equations are very formal, involving functional derivatives, and plotting their solution is typically as hard as solving a general non-Markovian open-system evolution. There are, of course, quite a few cases where the equations can be solved [23–27] as well as perturbative methods [28] to deal with a broader class of problems, but general non-perturbative approaches have so far been lacking.

In the following, we will introduce stochastic Schrödinger equations as unravelings of non-Markovian open-system dynamics making an extensive use of the general framework introduced recently by Diósi and Ferraldi [29]. Yet, our objective will not primarily be to find a numerically efficient way to compute the open-system evolution: we will be interested in the stochastic pure state trajectories themselves, having in mind their broader range of applications.

II. GENERAL FRAMEWORK

We consider an open quantum system evolving according to a general Gaussian Master Equation (GME), one of the broadest non-Markovian generalization of the Lindblad equation that is analytically tractable. We suppose the system has a proper Hamiltonian H_0 and will use the interaction picture for all operators $\hat{O}(t) = e^{iH_0 t} \hat{O} e^{-iH_0 t}$. The GME for the density matrix in interaction picture can then be written as a time ordered exponential [29]:

$$\begin{aligned} \rho(t) &= \Phi_t \cdot \rho(0) \\ &= \mathcal{T} \exp \left\{ \int_0^t \int_0^\tau d\tau ds D_{ij}(\tau, s) \left[\hat{A}_L^j(s) \hat{A}_R^i(\tau) \right. \right. \\ &\quad \left. \left. - \theta_{\tau s} \hat{A}_L^i(\tau) \hat{A}_L^j(s) - \theta_{s\tau} \hat{A}_R^j(s) \hat{A}_R^i(\tau) \right] \right\} \rho(0) \end{aligned} \quad (1)$$

where \mathcal{T} is the time ordering operator, $\{\hat{A}^k\}_{1 \leq k \leq n}$ are arbitrary system Hermitian operators, $D_{ij}(\tau, s)$ is a complex positive semi-definite kernel, $\theta_{\tau s} = \theta(\tau - s)$ is the Heaviside function, and we have used summation on repeated indices as well as the left-right notation for super-

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operators:

$$\hat{A}_L \rho = \hat{A} \rho ; \quad \hat{A}_R \rho = \rho \hat{A} .$$

At least if D is time translation invariant, equation (1) can be obtained from the linear coupling of the system with a general bosonic bath, in which case D can be related to the field two-point correlation functions [29]. It is also an equivalent operator rewriting of the well known quadratic Feynman-Vernon influence functional for systems linearly coupled to harmonic oscillators [30], a representation used *e.g.* by Hu, Paz and Zhang [31, 32] for the Quantum Brownian Motion and which can be derived from a vast class of microscopic models [33]. Here, we are not interested in the open system dynamics *per se* and thus step back from its implementation details to take the very general equation (1) as our starting point.

A stochastic unraveling of equation (1) is a set of pure state trajectories $|\psi_\xi(t)\rangle$ indexed by a set of random fields

$\xi = \{\xi_k\}_{1 \leq k \leq n}$ such that:

$$\rho(t) = \mathbb{E}_\xi [|\psi_\xi(t)\rangle \langle \psi_\xi(t)|] , \quad (2)$$

where $\mathbb{E}_\xi[\cdot] = \int \cdot d\mu_o(\xi)$ denotes averaging over the set of complex stochastic fields ξ . The interest of this rewriting is that it decouples the left and right parts of the time ordered exponential Φ_t of equation (1), a trick which is sometimes called a Hubbard-Stratonovich transformation. Let us now find an explicit candidate for $|\psi_\xi(t)\rangle$. Following *e.g.* [29], we first introduce a set of Gaussian complex fields of zero average and thus fully characterized by its following two point correlation functions:

$$\begin{aligned} \mathbb{E}_\xi [\xi_i(\tau) \xi_j^*(s)] &= C_{ij}(\tau, s) \\ \mathbb{E}_\xi [\xi_i(\tau) \xi_j(s)] &= S_{ij}(\tau, s) \end{aligned} \quad (3)$$

where S is the *relation* function, a symmetric complex kernel which can be chosen freely provided the full correlation kernel is positive semi-definite.

For two sets of fields a_t^k and b_t^k , the following generalized characteristic function is obtained by Gaussian integration:

$$\mathbb{E}_\xi \left[\exp \left\{ -i \int_0^t ds (a_s^k \xi_k(s) - b_s^k \xi_k^*(s)) \right\} \right] = \exp \left\{ \int_0^t \int_0^t d\tau ds C_{ij}(\tau, s) a_\tau^i b_s^j - \frac{S_{ij}(\tau, s) a_\tau^i a_s^j + S_{ij}^*(\tau, s) b_\tau^i b_s^j}{2} \right\} , \quad (4)$$

an equality that can be further generalized for a 's and b 's promoted to operators provided both sides are time ordered:

$$\mathbb{E}_\xi \left[\mathcal{T} \exp \left\{ -i \int_0^t ds (\hat{a}_s^k \xi_k(s) - \hat{b}_s^k \xi_k^*(s)) \right\} \right] = \mathcal{T} \exp \left\{ \int_0^t \int_0^t d\tau ds C_{ij}(\tau, s) \hat{a}_\tau^i \hat{b}_s^j - \frac{S_{ij}(\tau, s) \hat{a}_\tau^i \hat{a}_s^j + S_{ij}^*(\tau, s) \hat{b}_\tau^i \hat{b}_s^j}{2} \right\} . \quad (5)$$

The similarity between the r.h.s of (5) and (1) suggests to identify $\mathbb{E}_\xi[|\psi_\xi\rangle \langle \psi_\xi|]$ with the l.h.s of (5) with $\hat{a}_s^k = \hat{A}_L^k(s)$, $\hat{b}_s^k = \hat{A}_R^k(s)$ and $C_{ij}(\tau, s) = D_{ij}(\tau, s)$. Actually, this does not fully do the trick, a counter term remains, and one sees following [29] that the correct prescription is:

$$\begin{aligned} |\psi_\xi(t)\rangle &= \hat{G}_\xi(t) |\psi_0\rangle \\ &:= \mathcal{T} \exp \left\{ -i \int_0^t ds \hat{A}^k(s) \xi_k(s) \right. \\ &\quad \left. - \int_0^t \int_0^t d\tau ds \theta_{\tau s} [D - S]_{ij}(\tau, s) \hat{A}^i(\tau) \hat{A}^j(s) \right\} |\psi_0\rangle , \end{aligned} \quad (6)$$

which fulfills the unraveling condition (2). Equation (6) can subsequently be written in differential form to yield a non-Markovian stochastic Schrödinger equation:

$$\begin{aligned} \frac{d}{dt} |\psi_\xi(t)\rangle &= -i \hat{A}^i(t) [\xi_i(t) \\ &\quad + \int_0^t ds [D - S]_{ij}(t, s) \frac{\delta}{\delta \xi_j(s)}] |\psi_\xi(t)\rangle . \end{aligned} \quad (7)$$

To our knowledge, this equation is the most general *linear* non-Markovian stochastic Schrödinger equation ever

proposed [29]. Unfortunately, equation (7) is quite formal unless it is possible to write the functional derivative ¹ as a simple local operator acting on $|\psi_\xi(t)\rangle$.

III. MAIN RESULT

The core objective of this article is to show how the solutions of (7) can nonetheless be computed in the general case by reusing a stochastic unraveling trick, *i.e.* by writing this time:

$$|\psi_\xi(t)\rangle = \mathbb{E}_\eta [|\psi_{\xi, \eta}(t)\rangle] \quad (8)$$

where η is an auxiliary set of classical Gaussian fields. More precisely, we can try to write the evolution operator of (6) in the following way:

$$\hat{G}_\xi(t) = \mathbb{E}_\eta \left[\mathcal{T} \exp \left\{ -i \int_0^t ds \hat{A}^k(s) [\xi_k(s) + \eta_k(s)] \right\} \right] . \quad (9)$$

¹ The reader puzzled by the rigorous definition of the functional derivative can as well use (6) in all situations.

Using again the Gaussian integration formula (5), one sees that the new unraveling condition (8) is satisfied provided η is a set of Gaussian fields with zero mean and two-point correlation functions given by:

$$\begin{aligned}\mathbb{E}_\eta[\eta_i(\tau)\eta_j(s)] &= K_{ij}(\tau, s) \\ \mathbb{E}_\eta[\eta_i(\tau)\eta_j^*(s)] &= J_{ij}(\tau, s)\end{aligned}\quad (10)$$

with:

$$K_{ij}(\tau, s) = \theta_{\tau s} [D - S]_{ij}(\tau, s) + \theta_{s\tau} [D - S]_{ji}(s, \tau) \quad (11)$$

and where the other correlation function J can be chosen freely provided the total kernel Γ :

$$\Gamma = \begin{pmatrix} J & K \\ K^* & J^* \end{pmatrix} \quad (12)$$

is positive semi-definite².

Equation (9) can be written in an explicit linear differential form free of functional derivatives:

$$\frac{d}{dt}|\psi_{\xi, \eta}(t)\rangle = -i\hat{A}^k(t)[\xi_k(t) + \eta_k(t)]|\psi_{\xi, \eta}(t)\rangle. \quad (13)$$

This latter equation, together with its unraveling interpretation (8) is the main result of this article. The evolution given by equation (13) is *time-local* in the sense that once the random fields ξ and η are fixed, the state can be evolved without reference to the past. Although our interest was primarily in the stochastic pure state $|\psi_\xi\rangle$ itself, we can write the open-system density matrix as a double average over our successive unravelings (2) and (8):

$$\rho(t) = \mathbb{E}_\xi \left[\mathbb{E}_\eta [|\psi_{\xi, \eta}(t)\rangle] \mathbb{E}_\eta [\langle \psi_{\xi, \eta}(t)|] \right]. \quad (14)$$

This can be written equivalently:

$$\rho(t) = \mathbb{E}_{\xi, \eta^{(1)}, \eta^{(2)}} [|\psi_{\xi, \eta^{(1)}}(t)\rangle \langle \psi_{\xi, \eta^{(2)}}(t)|], \quad (15)$$

where $\eta^{(1)}$ and $\eta^{(2)}$ are independent. This is the two state unraveling proposal of Stockburger and Grabert [34, 35]. We have thus found a connection between the standard stochastic pure state representations and the more exotic two state vector method used in numerical approaches to open-systems. This allows us to identify at least part of the freedom in the noise present in this latter method as coming from the kernel S which encodes different stochastic Schrödinger evolutions corresponding to the same open-system evolution. We can further risk the following heuristic interpretation of the two noises. The noise ξ is classical in the sense that it is averaged over at the density matrix level. It is also classical in the sense that it can be measured, each realization of a trajectory corresponding to a possible measurement result. The noise η , on the other hand, is quantum or coherent as all the possible contributions are summed over coherently at the pure state level.

² For a kernel K given by equation (11), there always exists a kernel J such that Γ is positive semi-definite. The existence of a random field η verifying (10) is then a consequence of the Bochner-Minlos theorem.

IV. NORM PRESERVING UNRAVELINGS

The linear stochastic differential equation (7) does not preserve the norm of the state vector $|\psi_\xi\rangle$. Normalized pure states are usually preferred in foundations but also for numerics: the norm of $|\psi_\xi\rangle$ typically diffuses and for large times, most trajectories give a vanishing contribution to the average (2) while nearly all the weight is provided by rare events. Here, we shall not be primarily concerned by numerical efficiency but would nevertheless like to be able to compute the solutions of normalized NMSSE for their other uses in measurement theory and in foundations.

To obtain a norm preserving evolution from the linear one, one needs to define a normalized state $|\tilde{\psi}_\xi\rangle$:

$$|\tilde{\psi}_\xi\rangle(t) = \frac{|\psi_\xi(t)\rangle}{\sqrt{\langle \psi_\xi(t)|\psi_\xi(t)\rangle}} \quad (16)$$

but also to introduce a new “cooked” (or Girsanov transformed) probability measure:

$$d\mu_t(\xi) = \langle \psi_\xi(t)|\psi_\xi(t)\rangle d\mu_o(\xi) \quad (17)$$

which insures that the unraveling condition $\rho(t) = \mathbb{E}_\xi [|\tilde{\psi}_\xi(t)\rangle \langle \tilde{\psi}_\xi(t)|]$ —where \mathbb{E}_ξ^t is the expectation value taken with the new measure μ_t —is still valid. The ideal solution would be to find a way to sample $|\tilde{\psi}_\xi\rangle$ directly. This is unfortunately not a trivial endeavour and the method we shall propose is arguably less appealing than in the linear case.

Let us first notice that, in most cases, being able to find solutions to the linear NMSSE is good enough. In the measurement context, the stochastic realization ξ is given: it is the measurement result³, and the fact that its probability distribution is non-Gaussian is irrelevant. One can simply use the linear equation to reconstruct the state from the measurement record and normalize at the very end. Another thing one may want to do is to compute certain expectation values with the Girsanov transformed probability measure $d\mu_t$. Again, this only requires to be able to solve the linear equation: one just needs to use the defining equation $\mathbb{E}_\xi^t[\cdot] = \mathbb{E}_\xi^\circ[\cdot \langle \psi_\xi(t)|\psi_\xi(t)\rangle]$. Consequently, for all practical purposes, being able to solve the linear NMSSE is good enough, even if it may be numerically inefficient.

Still, one may wish to be able to sample from the norm preserving evolution, if only to plot “typical” trajectories and get an intuition of the physics. Because the probability distribution of ξ is non-Gaussian in the normalized case, the task is not trivial. Yet, when direct sampling seems too hard, it is always possible to use indirect sampling methods [36], which in the situation we are interested in are quite straightforward.

³ The latter is understood again as a single shot record and not as a real-time measurement trajectory [19].

We would typically like to do rejection sampling, *i.e.* keep a given trajectory $|\psi_\xi\rangle$, initially generated with the measure $d\mu_\circ$, if a random number in $[0, 1]$ is smaller than $\langle\psi_\xi(t)|\psi_\xi(t)\rangle \max_\zeta[\langle\psi_\zeta(t)|\psi_\zeta(t)\rangle]^{-1}$. Unfortunately, the latter maximum does not exist, $\langle\psi_\xi(t)|\psi_\xi(t)\rangle$ is unbounded. We thus need to use a slight extension of rejection sampling which is but a trivial instantiation of the Metropolis algorithm.

We define a Markov chain $X_n = \xi^{(n)}$ of complete noise trajectories (and implicitly associate their corresponding pure states). Assuming the chain is defined at step n (unrelated to the physical time t), we draw a new noise trajectory ξ independently from the Gaussian measure $d\mu_\circ$, and compute the corresponding state $|\psi_\xi\rangle$ with the linear equation. We then update the Markov chain in the following way:

$$X_{n+1} = \begin{cases} \xi & \text{with probability } p_{n+1} \\ X_n & \text{with probability } 1 - p_{n+1} \end{cases} \quad (18)$$

with $p_{n+1} = \min(1, \langle\psi_\xi(t)|\psi_\xi(t)\rangle / \langle\psi_{\xi^{(n)}}(t)|\psi_{\xi^{(n)}}(t)\rangle)$. This gives a Markov chain with the transition probabilities:

$$d\mathbb{P}[\xi \rightarrow \zeta] = \min\left(1, \frac{\langle\psi_\zeta(t)|\psi_\zeta(t)\rangle}{\langle\psi_\xi(t)|\psi_\xi(t)\rangle}\right) d\mu_\circ(\zeta), \quad (19)$$

from which it is then easy to read that the invariant measure is $d\mu_t$. Hence, the Markov chain X_n samples the noise trajectories with the correct non-Gaussian probability measure. The method is not too inefficient in this context because the samples are independent before the rejection step. This final step is indeed the only one that correlates the final outcomes through the possible repetition of the same realization. In practice, it is even possible to save some computing time at each step by drawing a random real number r uniformly distributed between 0 and 1 *before* computing $|\psi_\xi\rangle$. As the approximation of $|\psi_\xi\rangle$ is progressively refined through the addition of more $|\psi_{\xi,\eta}\rangle$, one can compare the approximated norm to $q_n \times r$ and stop further refining if it is already clear that the sample is unlikely to be kept.

V. EXAMPLE

We now illustrate our method on an example where the stochastic Schrödinger equation is fully explicit. For that matter, we consider a single Hermitian operator \hat{A} commuting with H_0 (s.t. $\hat{A}(t) = \hat{A}$) and purely imaginary noise, *i.e.* $S = -D$, which gives the following stochastic Schrödinger equation:

$$\frac{d}{dt}|\psi_\xi(t)\rangle = -i\hat{A}\left[\xi(t) + 2\int_0^t ds D(t,s)\frac{\delta}{\delta\xi(s)}\right]|\psi_\xi(t)\rangle. \quad (20)$$

For a given realization of ξ , $|\psi_\xi\rangle$ obeys an explicit differential equation. Indeed, using the integral form (6), we

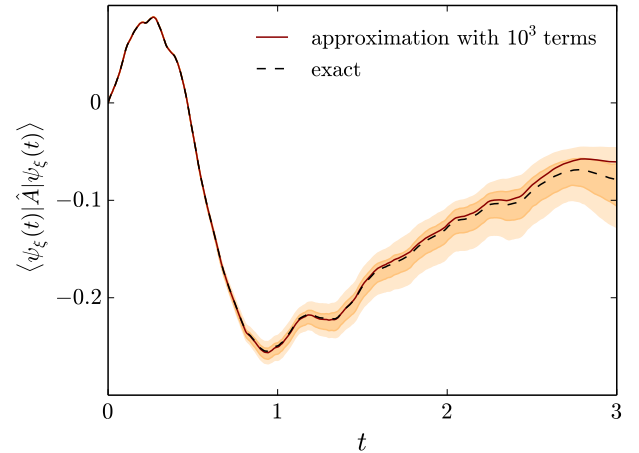


FIG. 1. Snapshot of a linear trajectory $|\psi_\xi\rangle$ for a random realization of ξ . The shaded areas indicate the zones where 50% ($\simeq 0.5\sigma$) and 85% ($\simeq 1\sigma$) of the approximate trajectories would lie. The exact trajectory is obtained from equation (20) while the approximate trajectory is obtained from (8) and the estimation $|\psi_\xi\rangle \simeq \frac{1}{N} \sum_{n=1}^N |\psi_{\xi,\eta}\rangle$ with $N = 10^3$ independent realizations of η and the same fixed ξ . The number of realizations is voluntarily left small to make the estimate of the error visible as the latter decreases $\propto N^{-1/2}$.

can replace the functional derivative:

$$\frac{\delta}{\delta\xi(s)}|\psi_\xi(t)\rangle = -i\hat{A}|\psi_\xi(t)\rangle. \quad (21)$$

This example thus offers a nice testbed for our stochastic approach. Numerical results for $\hat{A} = \text{diag}(1, 0, -1)$ and $D(t, 0) = e^{-t}$ are shown in figure 1. In this example, the relaxation timescale responsible for the non-Markovianity and the timescale of the system-bath coupling are both of order 1 and we would thus be deep in the non-Markovian regime had the system Hamiltonian not been trivial. Our method is efficient for evolution times of the order of the this second timescale and becomes exponentially expensive for larger times as one would expect from the fact that the norm of $|\psi_{\xi,\eta}\rangle$ diffuses and converges almost surely to zero.

We also test our Metropolis method to sample solutions of the norm-preserving non-linear NMSSE (see figure 2). We observe that the typical trajectories for the initial Gaussian and Metropolis sampled measures widely differ. This means that sampling from the correct non-Gaussian measure is the only way to get a reasonably good intuition of the physics (although, as we argued, all measurable quantities can be computed with the linear NMSSE). This is also the sign, rather unfortunately, that our rejection sampling method is expensive as it requires finding and giving weight to trajectories that are atypical with the Gaussian measure. Again, this cost increases exponentially with time as it is related to the fact that the norm of $|\psi_\xi(t)\rangle$ goes to zero exponentially quickly for typical trajectories. Even if direct sampling remains out

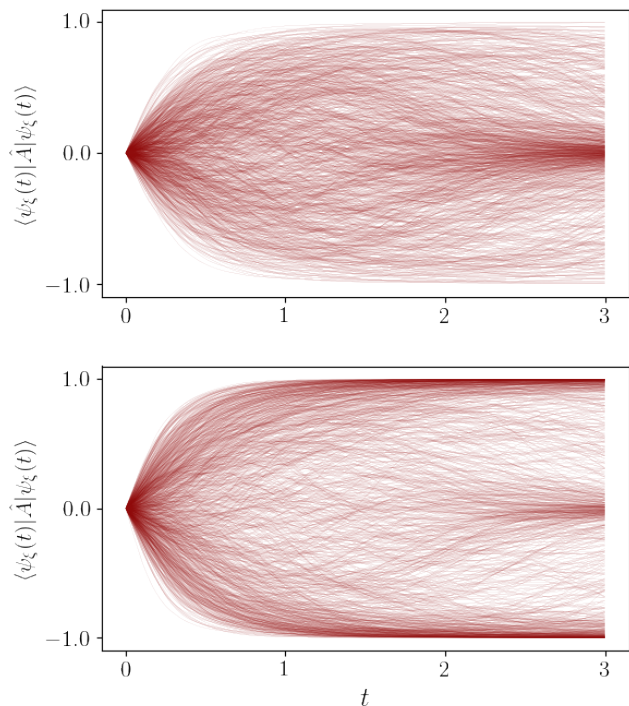


FIG. 2. Illustration of the change of measure: 10^3 normalized quantum trajectories $|\tilde{\psi}_\xi\rangle$ where ξ is sampled with the (incorrect) raw Gaussian measure $d\mu_o$ on the upper plot and (correct) non-Gaussian measure $d\mu_t$ on the lower plot. The latter is obtained using the Metropolis Markov chain, with a relaxation time of 10^3 iterations between each sample. The initial condition is $|\tilde{\psi}_\xi(0)\rangle = 3^{-1/2}(1, 1, 1)$ such that one expects $\langle \tilde{\psi}_\xi(t) | \hat{A} | \tilde{\psi}_\xi(t) \rangle$ to converge to -1 , 0 , or $+1$ for large time with equal probability.

of reach in the future, one may hope that new Metropolis sampling methods, smarter than the naive one we have proposed, could yield dramatic speed-ups.

VI. CONCLUSION

In this article, we have introduced a rewriting (or “unraveling”) of the solutions of formal NMSSE as averages over the solutions of explicit time-local stochastic differential equations. This new formulation may provide a basis for further analytical studies, notably as it provides an extremely simple new way to define NMSSE. More importantly, it immediately offers a method to compute numerically their solutions. Although we have proposed a heuristic interpretation of the quantum and classical character of the two noises involved, the auxiliary state $|\psi_{\xi,\eta}\rangle$ does not yet have a clear operational characterization. The latter would certainly help understand the freedom in the noise kernel J . An important limitation of this work is the lack of a direct extension to non-linear NMSSE (although we have presented a Metropolis sampling way out). Any advance in this direction would dramatically improve our ability to deal with non-Markovian open-systems numerically.

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